Argonne NATIONAL LABORATORY

TOWARDS PRACTICAL QUANTUM OPTIMIZATION AND MACHINE LEARNING

RUSLAN SHAYDULIN
Argonne National Laboratory

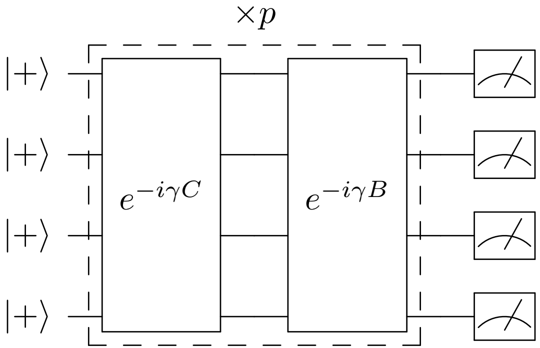
arXiv:2106.04410
arXiv:2111.05451

Nov 22, 2021

QUANTUM APPROXIMATE OPTIMIZATION ALGORITHM (QAOA)

- QAOA prepares a parameterized “trial” (ansatz) state of the form:

$$\begin{aligned}|\mathrm{QAOA}\rangle &= |\boldsymbol{\beta}, \boldsymbol{\gamma}\rangle \\ &= e^{-i\beta_p B} e^{-i\gamma_p C} \ldots e^{-i\beta_1 B} e^{-i\gamma_1 C} |+\rangle^{\otimes n}\end{aligned}$$



APPLICATION

Error Mitigation for QAOA by Leveraging Problem Symmetries

- Assume each gate is followed by 1-qubit noise with probability *p*
- **No advantage at depth p^{-1}** [1]

[1] arXiv:2009.05532

APPLICATION

Error Mitigation for QAOA by Leveraging Problem Symmetries

- Assume each gate is followed by 1-qubit noise with probability *p*
- **No advantage at depth p^{-1}** [1]

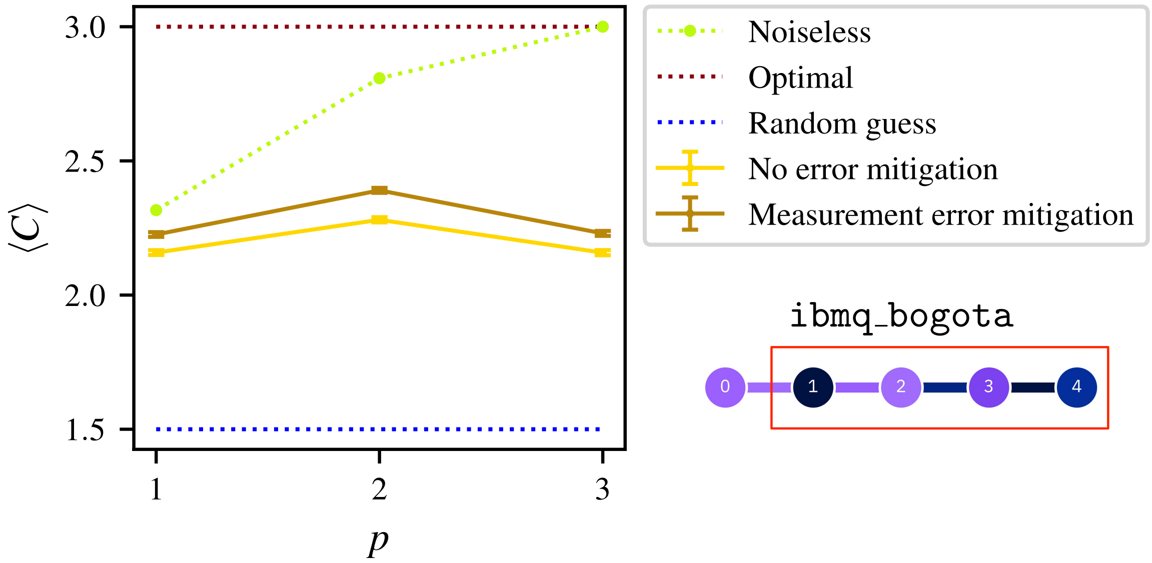
Some error mitigation is required for quantum advantage in optimization (and elsewhere, probably)

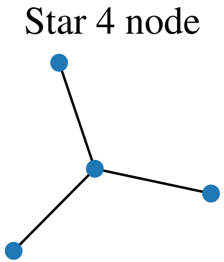
[1] arXiv:2009.05532

APPLICATION

Error Mitigation for QAOA by Leveraging Problem Symmetries

- In practice, no more than a a few layers of QAOA can be executed





ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

Theorem 1 *Consider a symmetry* $A \in S_{2^n}$ *acting as* $A|x\rangle = |a(x)\rangle, x \in \{0,1\}^n$ *s.t.* $[A, C] = 0 = [A, B]$. *Then solution probability amplitudes are invariant under this symmetry:*

$$\langle x \mid \boldsymbol{\beta}, \boldsymbol{\gamma} \rangle_p = \langle a(x) \mid \boldsymbol{\beta}, \boldsymbol{\gamma} \rangle_p, \quad \forall \boldsymbol{\beta}, \boldsymbol{\gamma}, p$$

ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

Theorem 1 *Consider a symmetry* $A \in S_{2^n}$ *acting as* $A|x\rangle = |a(x)\rangle, x \in \{0,1\}^n$ *s.t.* $[A, C] = 0 = [A, B]$*. Then solution probability amplitudes are invariant under this symmetry:*

$$\langle x \mid \boldsymbol{\beta}, \boldsymbol{\gamma} \rangle_p = \langle a(x) \mid \boldsymbol{\beta}, \boldsymbol{\gamma} \rangle_p, \quad \forall \boldsymbol{\beta}, \boldsymbol{\gamma}, p$$

And the QAOA state is stabilized by A*:*

$$A \left| \boldsymbol{\beta}, \boldsymbol{\gamma} \right\rangle_p = \left| \boldsymbol{\beta}, \boldsymbol{\gamma} \right\rangle_p, \quad \forall \boldsymbol{\beta}, \boldsymbol{\gamma}, p$$

ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

- The QAOA state is stabilized by A with eigenvalues ±1:

$$A\,|\boldsymbol{\beta},\boldsymbol{\gamma}\rangle_p = |\boldsymbol{\beta},\boldsymbol{\gamma}\rangle_p\,, \quad \forall\boldsymbol{\beta},\boldsymbol{\gamma},p$$

ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

- The QAOA state is stabilized by A with eigenvalues ±1:

$$A \left| \boldsymbol{\beta}, \boldsymbol{\gamma} \right\rangle_p = \left| \boldsymbol{\beta}, \boldsymbol{\gamma} \right\rangle_p , \quad \forall \boldsymbol{\beta}, \boldsymbol{\gamma}, p$$

- Therefore, projection onto the +1 eigenspace of A stabilizes the QAOA state:

$$M_A \left| \boldsymbol{\beta}, \boldsymbol{\gamma} \right\rangle_p = \frac{1}{2}(I + A) \left| \boldsymbol{\beta}, \boldsymbol{\gamma} \right\rangle_p = \left| \boldsymbol{\beta}, \boldsymbol{\gamma} \right\rangle_p , \quad \forall \boldsymbol{\beta}, \boldsymbol{\gamma}, p$$

ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

- The QAOA state is stabilized by A with eigenvalues ±1:

$$A\,|\boldsymbol{\beta},\boldsymbol{\gamma}\rangle_p = |\boldsymbol{\beta},\boldsymbol{\gamma}\rangle_p\,, \quad \forall \boldsymbol{\beta},\boldsymbol{\gamma},p$$

- Therefore, projection onto the +1 eigenspace of A stabilizes the QAOA state:

$$M_A\,|\boldsymbol{\beta},\boldsymbol{\gamma}\rangle_p = \frac{1}{2}(I+A)\,|\boldsymbol{\beta},\boldsymbol{\gamma}\rangle_p = |\boldsymbol{\beta},\boldsymbol{\gamma}\rangle_p\,, \quad \forall \boldsymbol{\beta},\boldsymbol{\gamma},p$$

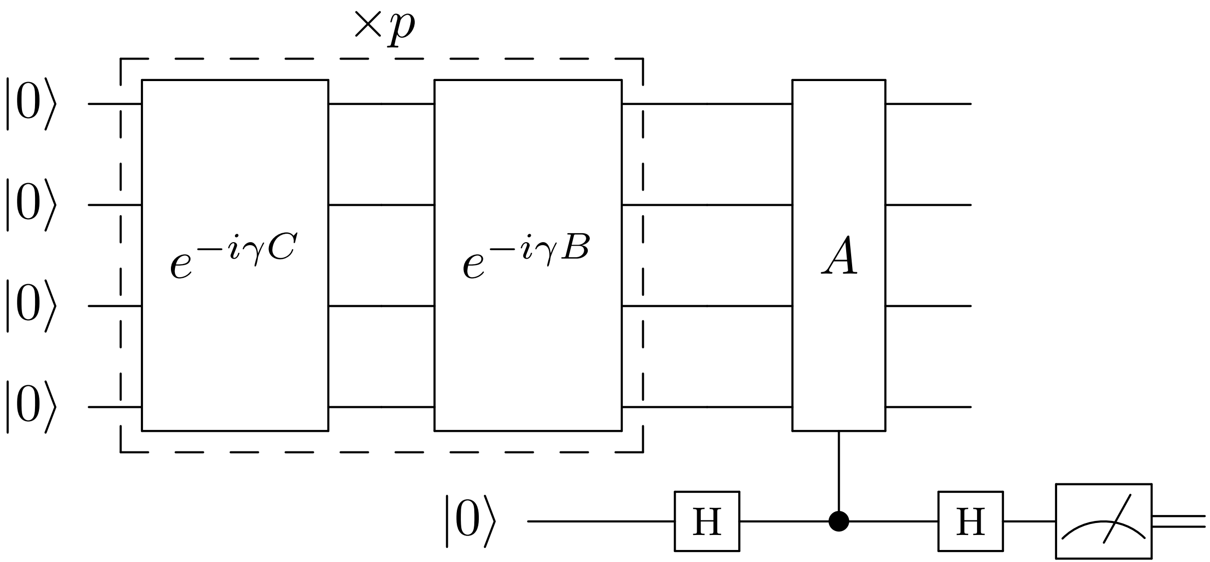
Idea: perform projector-valued measurement M_A on QAOA state.
If an error pushed the state out of the symmetry-protected subspace, the measurement would project the state back!

Proven to always **increases the overlap with true state**

ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

- Symmetry verification circuit:

$$M_A \left|\boldsymbol{\beta}, \boldsymbol{\gamma}\right\rangle_p = \left|\boldsymbol{\beta}, \boldsymbol{\gamma}\right\rangle_p, \quad \forall \boldsymbol{\beta}, \boldsymbol{\gamma}, p$$

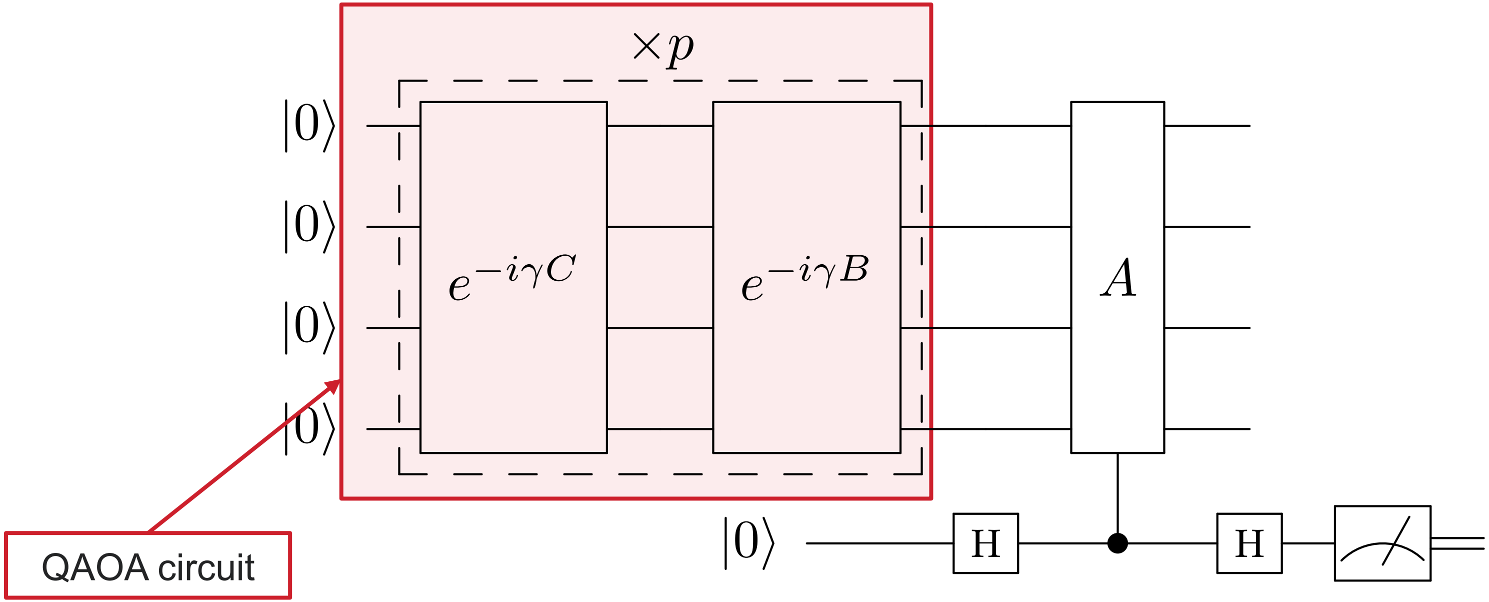


arXiv:2106.04410

ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

- Symmetry verification circuit:

$$M_A \left|\boldsymbol{\beta}, \boldsymbol{\gamma}\right\rangle_p = \left|\boldsymbol{\beta}, \boldsymbol{\gamma}\right\rangle_p, \quad \forall \boldsymbol{\beta}, \boldsymbol{\gamma}, p$$

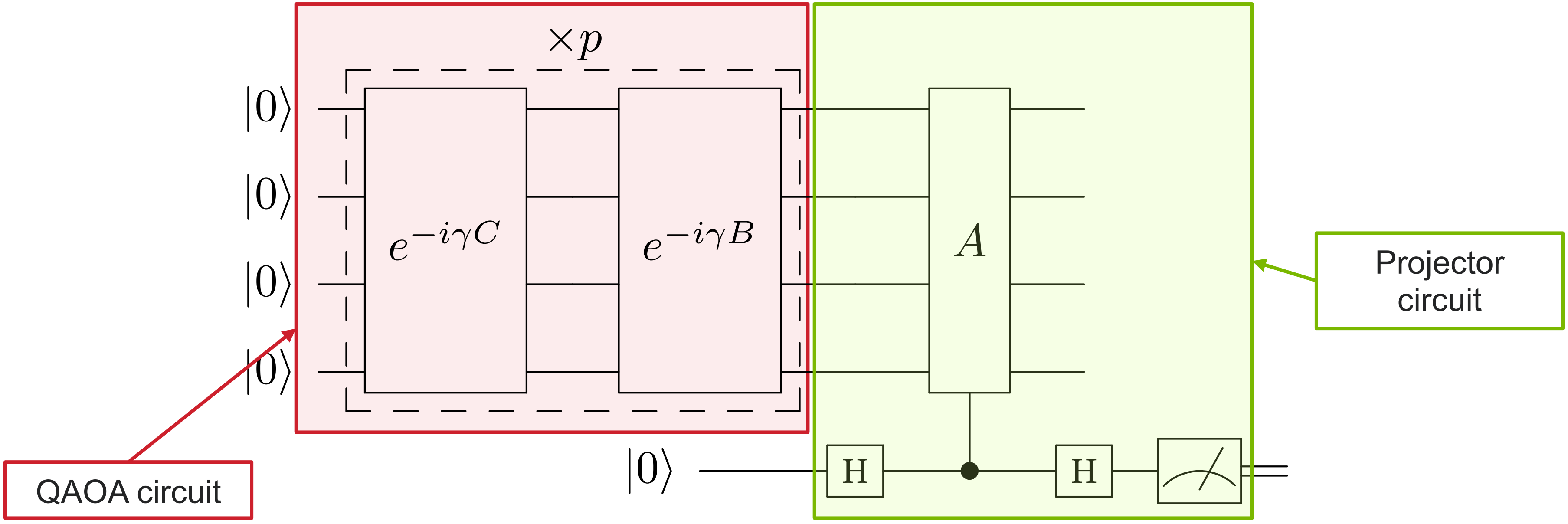


arXiv:2106.04410

ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

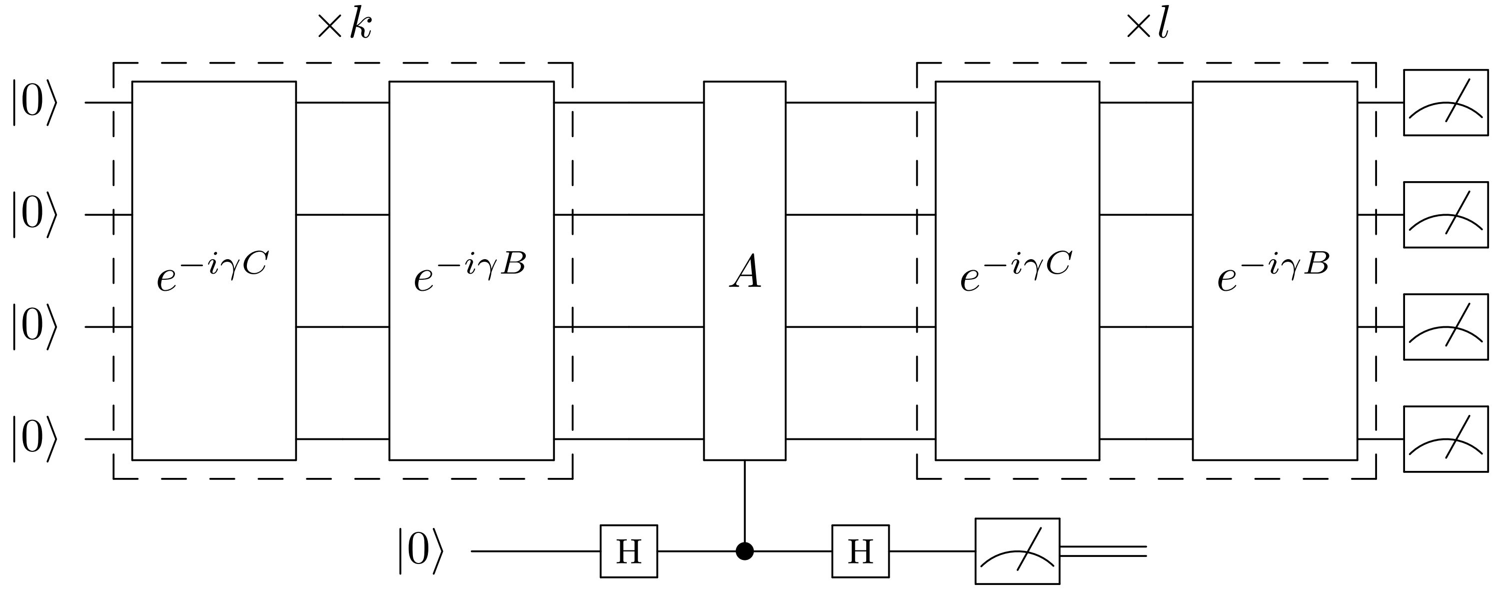
$$M_A |\boldsymbol{\beta}, \boldsymbol{\gamma}\rangle_p = |\boldsymbol{\beta}, \boldsymbol{\gamma}\rangle_p, \quad \forall \boldsymbol{\beta}, \boldsymbol{\gamma}, p$$

- Symmetry verification circuit:



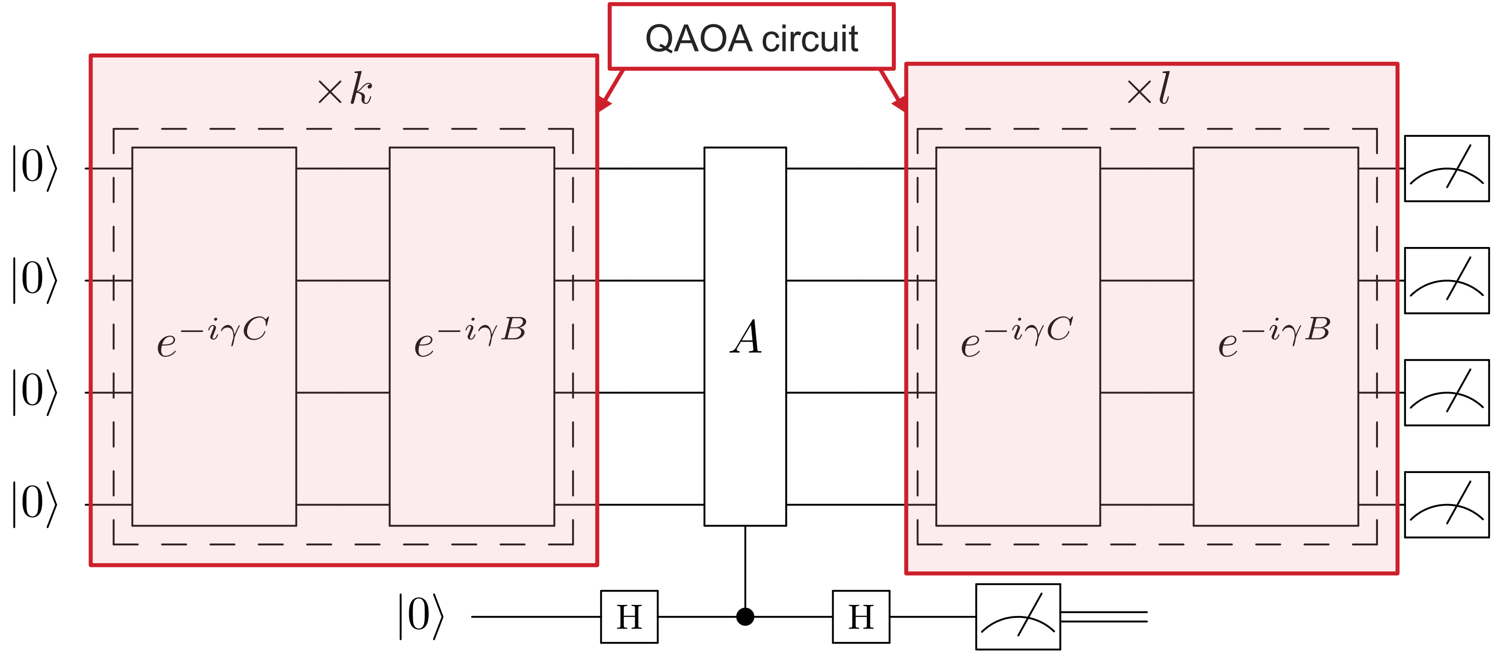
ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

- Symmetry verification need not be performed at the end of the circuit:



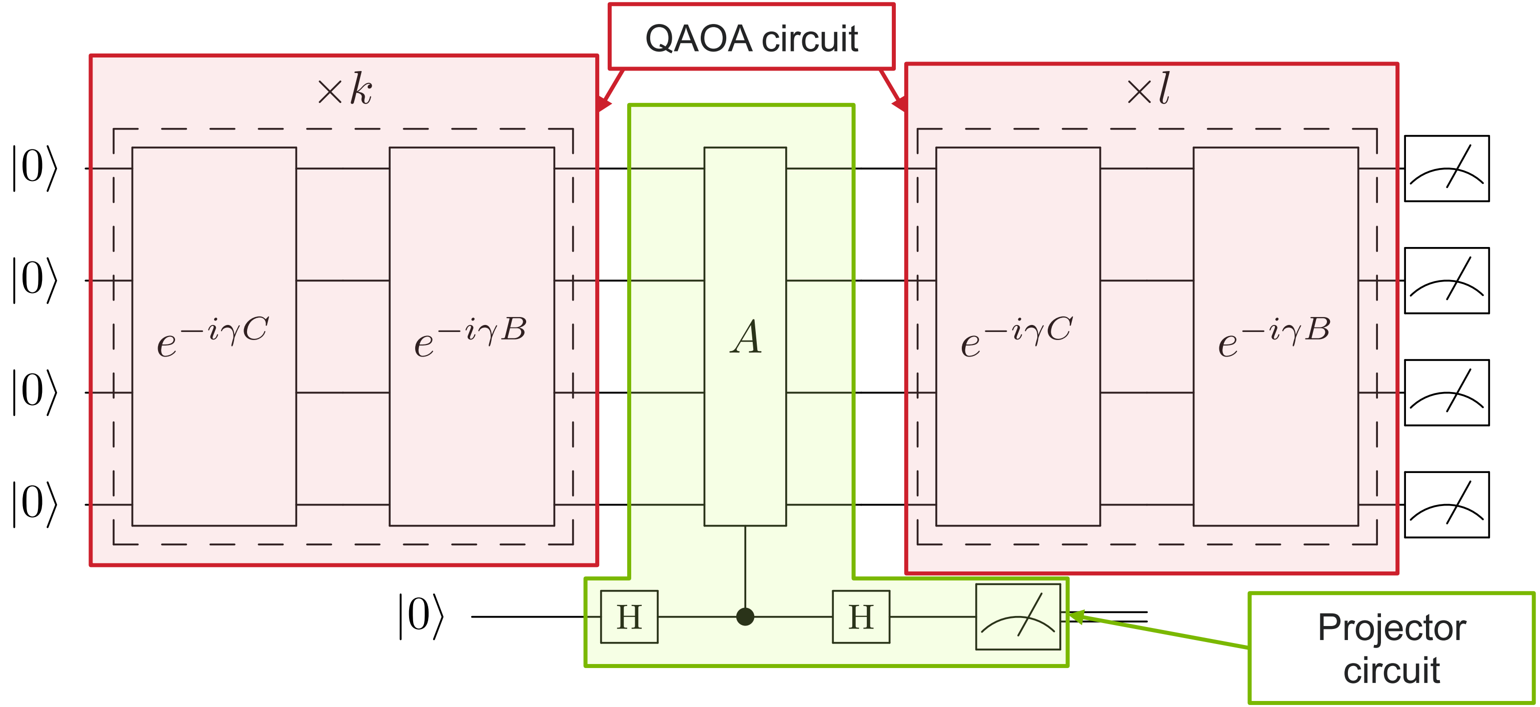
ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

- Symmetry verification need not be performed at the end of the circuit:



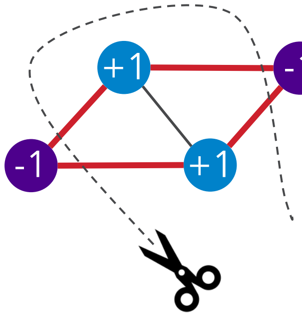
ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

- Symmetry verification need not be performed at the end of the circuit:



MAXCUT PROBLEM

- The goal of maximum cut is to split the set of vertices V of a graph into two disjoint parts such that the number of edges spanning two parts is maximized.



- MaxCut problem is encoded by the following Hamiltonian:

$$C_{\text{MaxCut}} = \frac{1}{2} \sum_{(u,v)\in E} (I - Z_u Z_v)$$

GRAPH SYMMETRIES AND QAOA

Corollary *Consider a graph with some label-independent objective function defined on its vertex configurations* $\{0,1\}^n$*. Suppose we know a subgroup of graph automorphisms* $\mathcal{A}_G \subseteq \mathrm{Aut}(G) \subseteq S_n \subset S_{2^n}$*. Then QAOA states satisfy:*

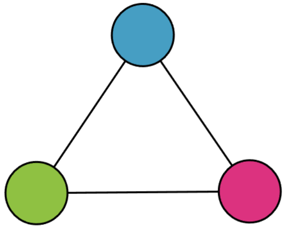
$$\forall x \in \{0,1\}^n,\ \ \forall p, \boldsymbol{\beta}, \boldsymbol{\gamma},\ \ \forall a_j \in \mathcal{A}_G \qquad \langle x \mid \boldsymbol{\beta}, \boldsymbol{\gamma} \rangle_p = \langle a_j(x) \mid \boldsymbol{\beta}, \boldsymbol{\gamma} \rangle_p$$

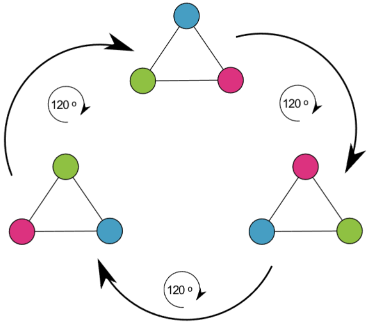
GRAPH SYMMETRIES AND QAOA

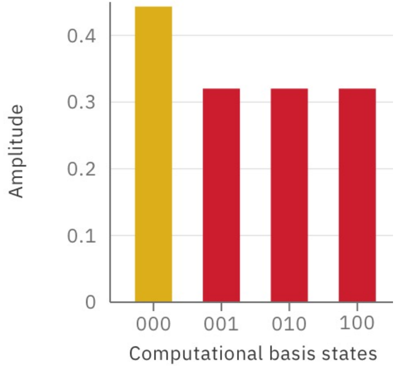
Corollary *Consider a graph with some label-independent objective function defined on its vertex configurations* $\{0,1\}^n$. *Suppose we know a subgroup of graph automorphisms* $\mathcal{A}_G \subseteq \mathrm{Aut}(G) \subseteq S_n \subset S_{2^n}$. *Then QAOA states satisfy:*

$$\forall x \in \{0,1\}^n, \;\; \forall p, \boldsymbol{\beta}, \boldsymbol{\gamma}, \;\; \forall a_j \in \mathcal{A}_G \qquad \langle x \mid \boldsymbol{\beta}, \boldsymbol{\gamma} \rangle_p = \langle a_j(x) \mid \boldsymbol{\beta}, \boldsymbol{\gamma} \rangle_p$$

Example

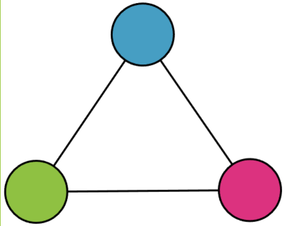


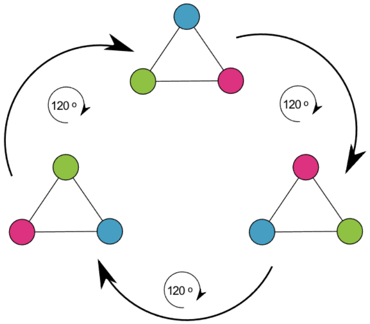


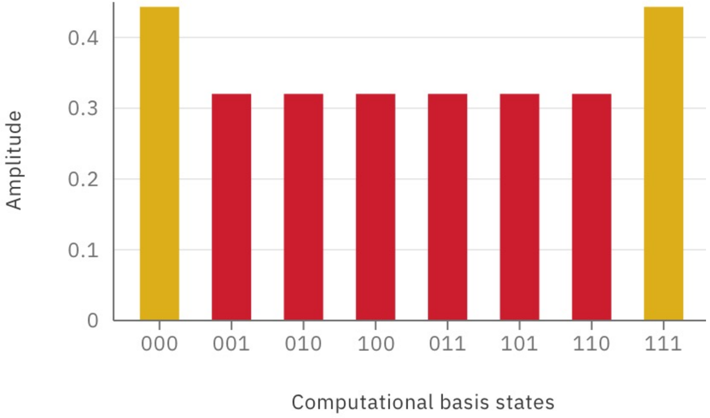


GRAPH SYMMETRIES AND QAOA

Cont'd

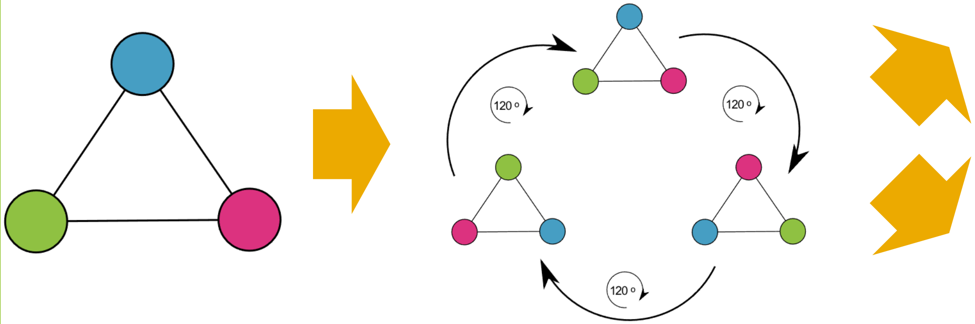


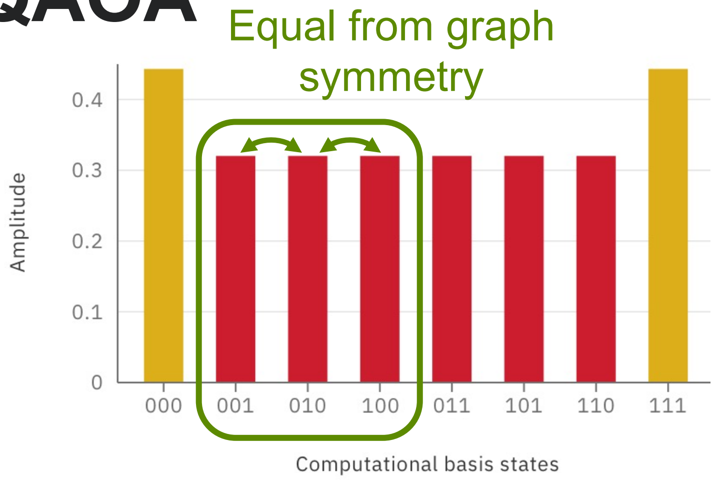




GRAPH SYMMETRIES AND QAOA

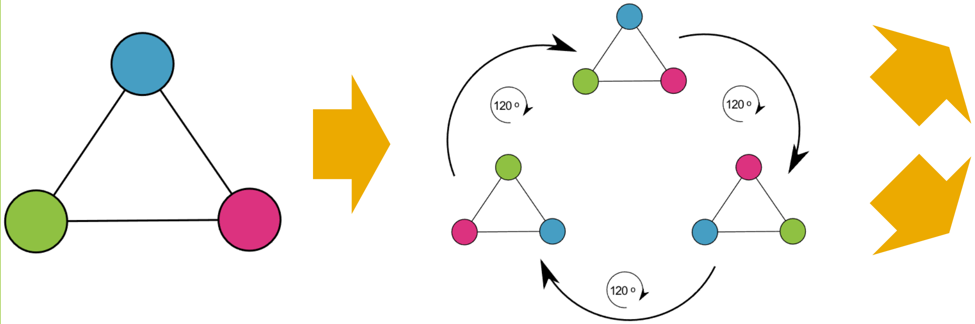
Cont'd

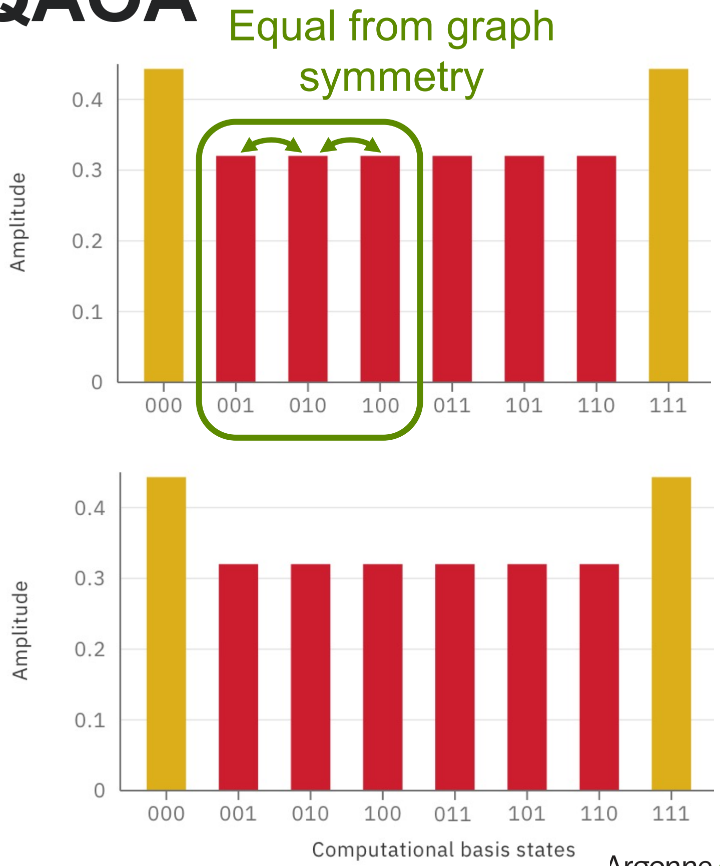




GRAPH SYMMETRIES AND QAOA

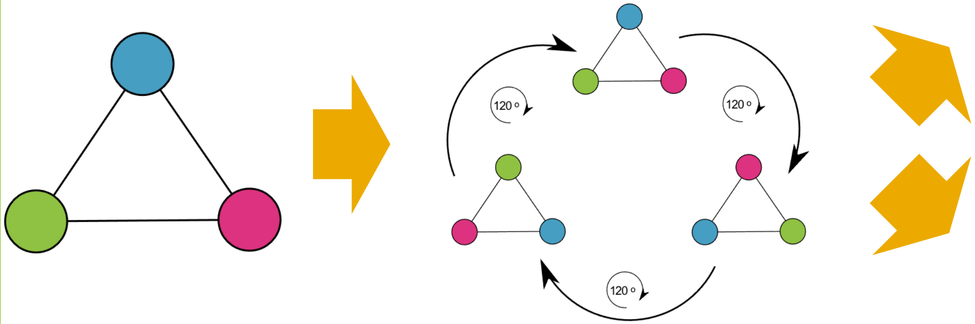
Cont’d

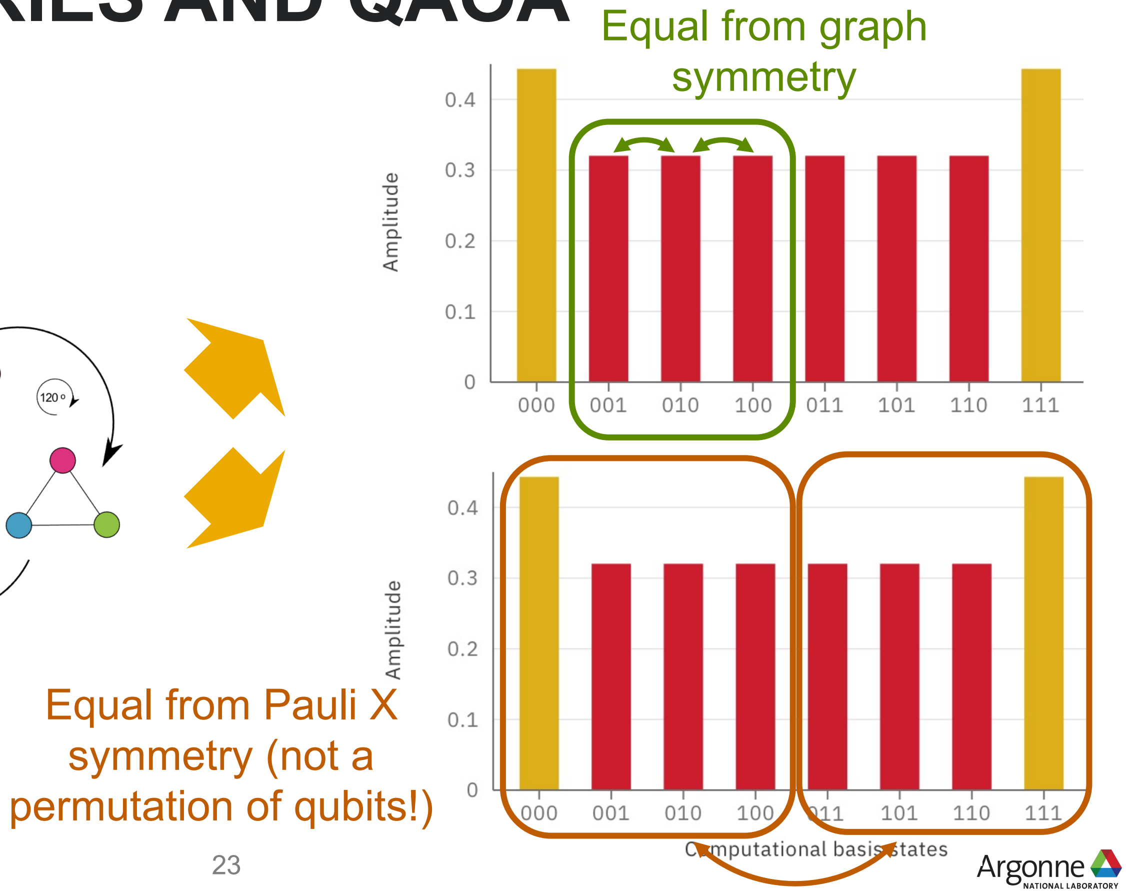




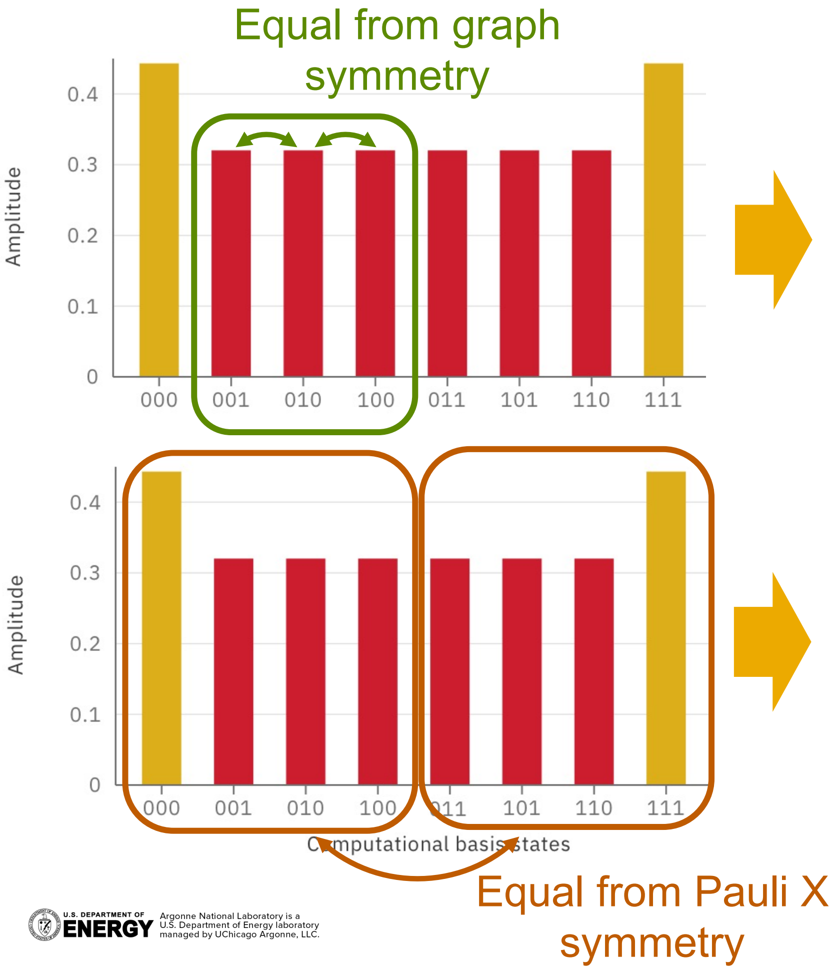
GRAPH SYMMETRIES AND QAOA

Cont'd





Application to MaxCut



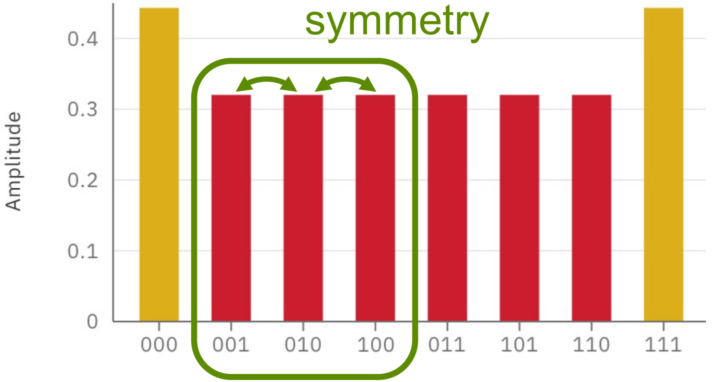
Symmetry operator

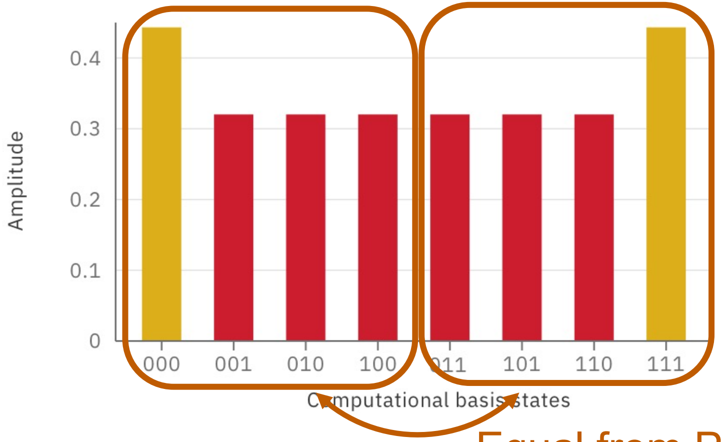
$$A = \mathrm{SWAP}_{j,k} \cdots \mathrm{SWAP}_{l,m}$$

$$A = \mathrm{X} \otimes \ldots \otimes \mathrm{X}$$

Application to MaxCut

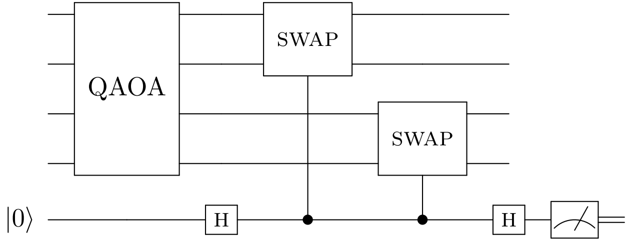
Equal from graph symmetry



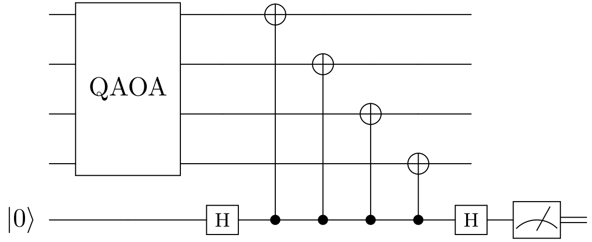


Equal from Pauli X symmetry

Symmetry verification circuit



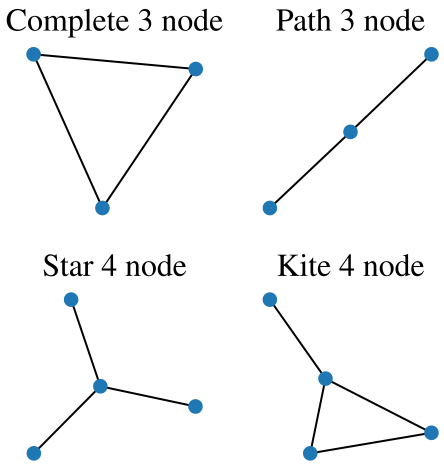
$$A = \mathrm{SWAP}_{j,k} \cdots \mathrm{SWAP}_{l,m}$$

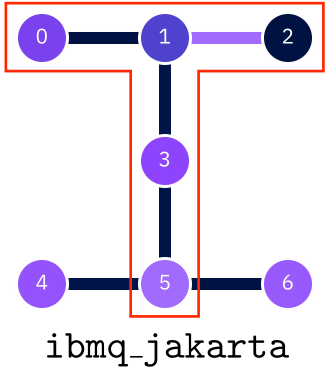


$$A = \mathrm{X} \otimes \ldots \otimes \mathrm{X}$$

ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

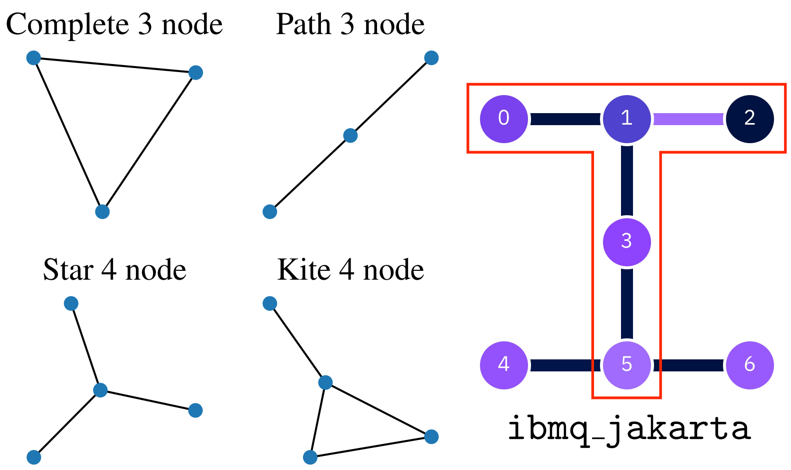
Experimental results

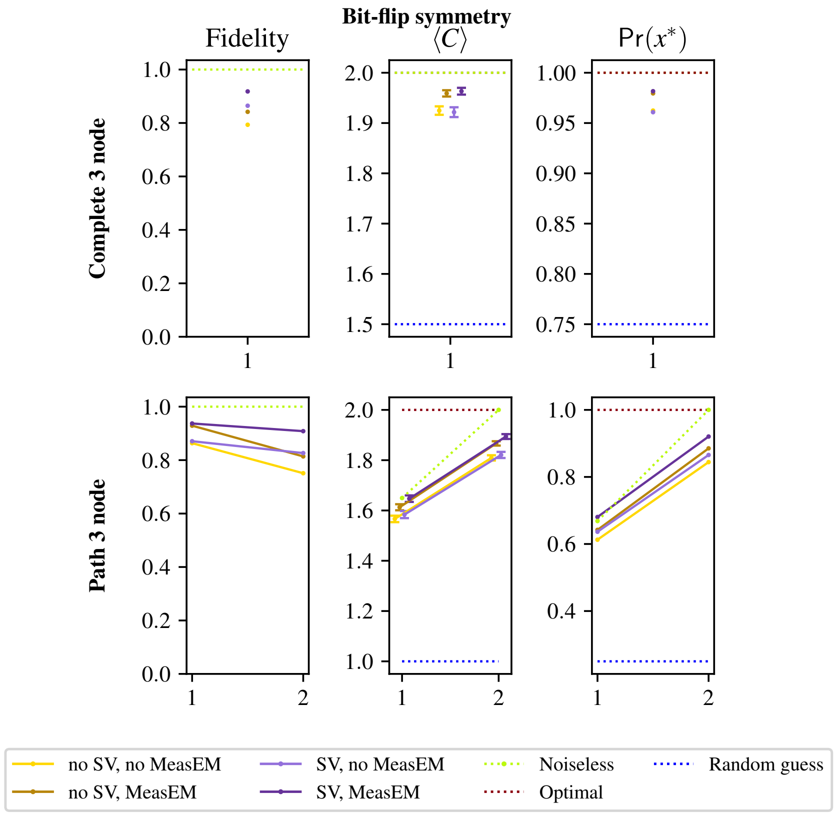




ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

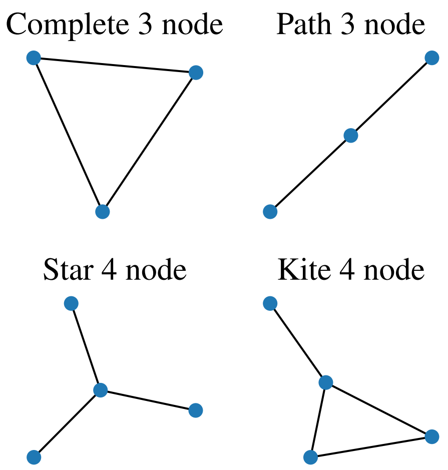
Experimental results

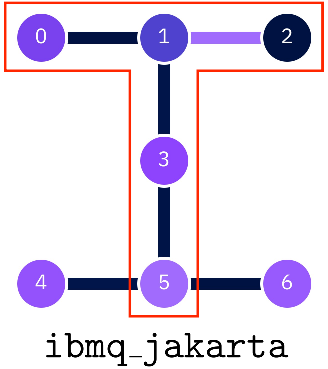


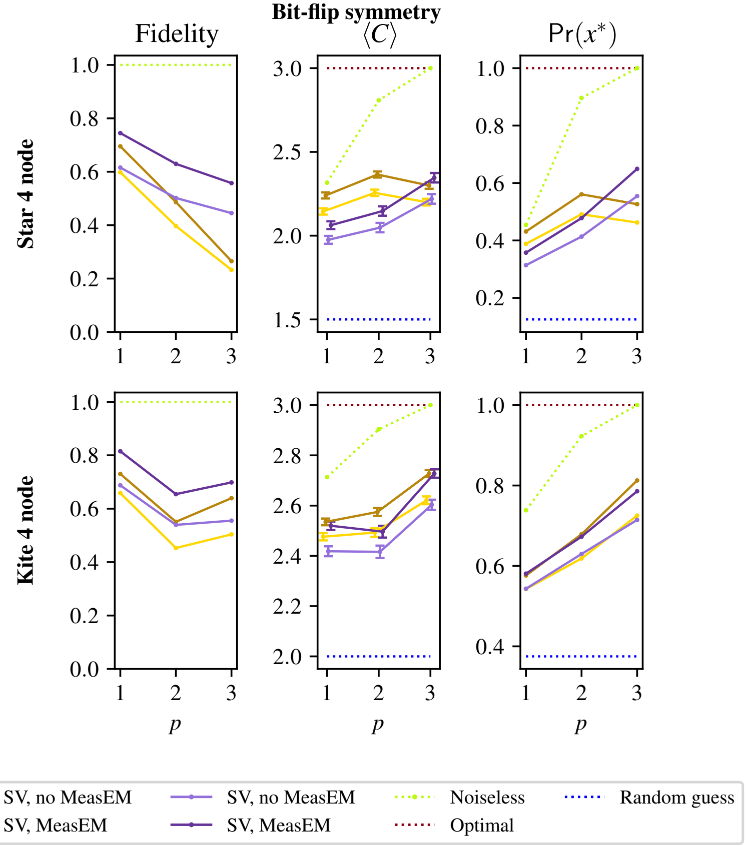


ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

Experimental results



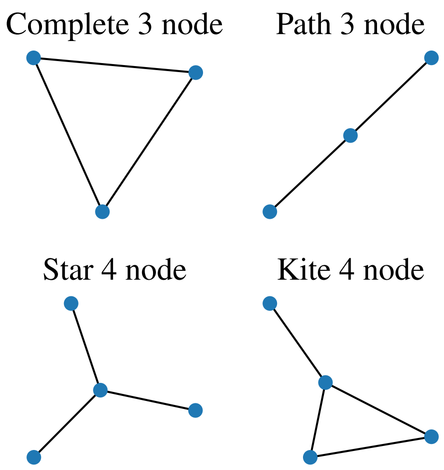


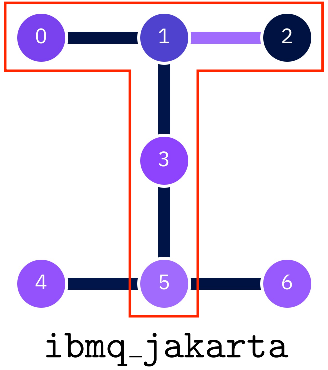


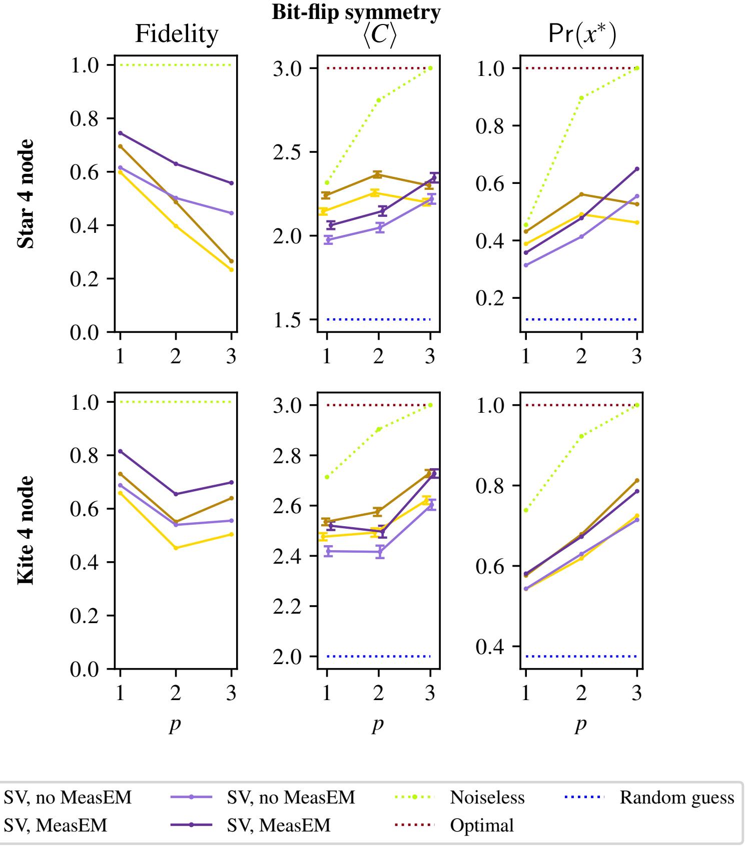
Fidelity improvement from bit-flip symmetry verification on all instances!

ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

Experimental results



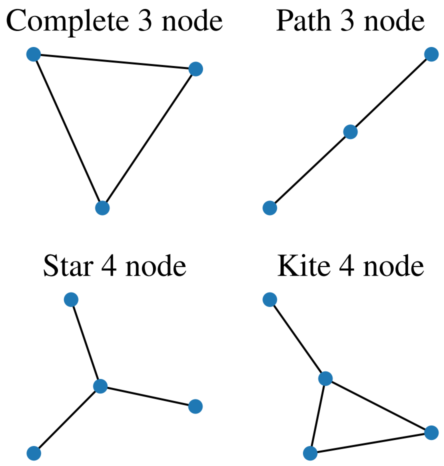


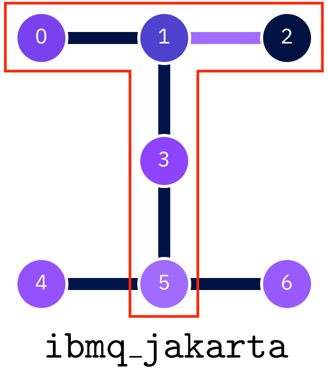


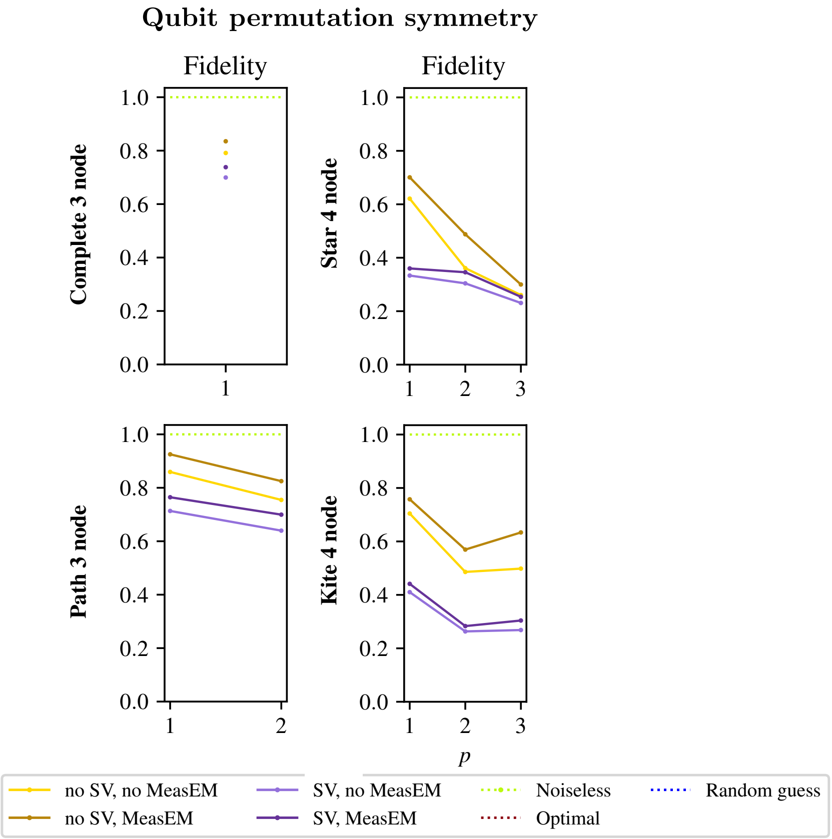
Fidelity improvement need not lead to objective value improvement

ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

Experimental results





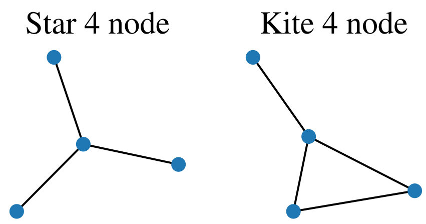


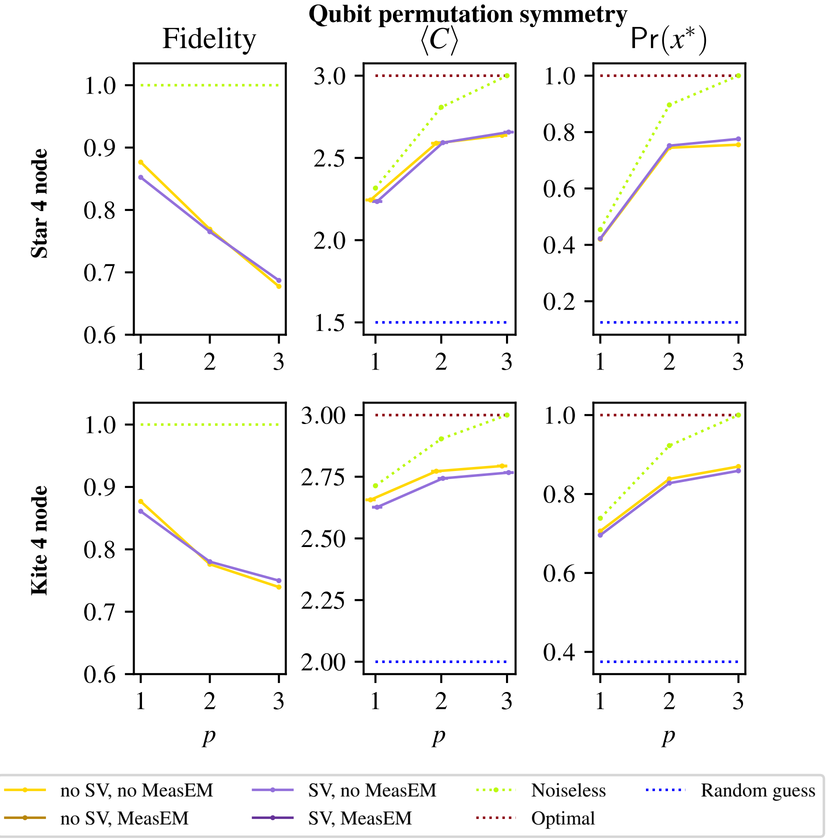
No fidelity improvement on hardware from qubit permutation symmetry verification

ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

Simulation results

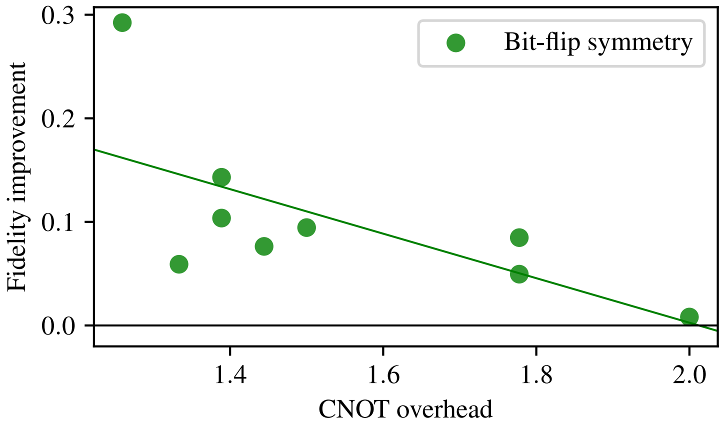
- Only depolarizing and thermal relaxation error
- Fidelity improvement in simulation shows the potential of the proposed methods

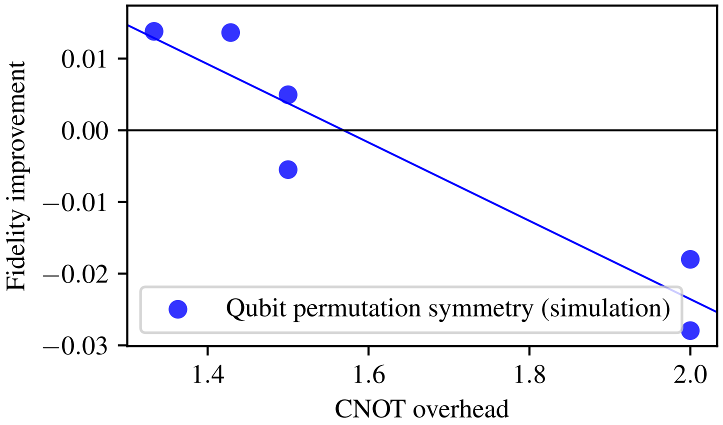




ERROR MITIGATION BY VERIFICATION OF THE OBJECTIVE FUNCTION SYMMETRIES

Overhead of symmetry verification

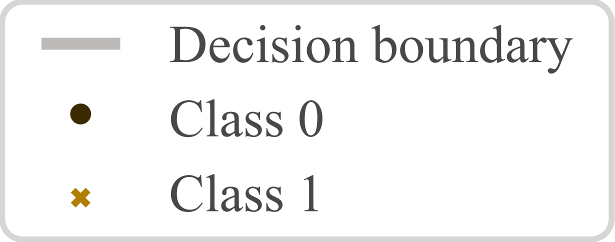




- Better compilation techniques (e.g. [1]) and better hardware connectivity reduce the overhead, leading to higher improvements in fidelity

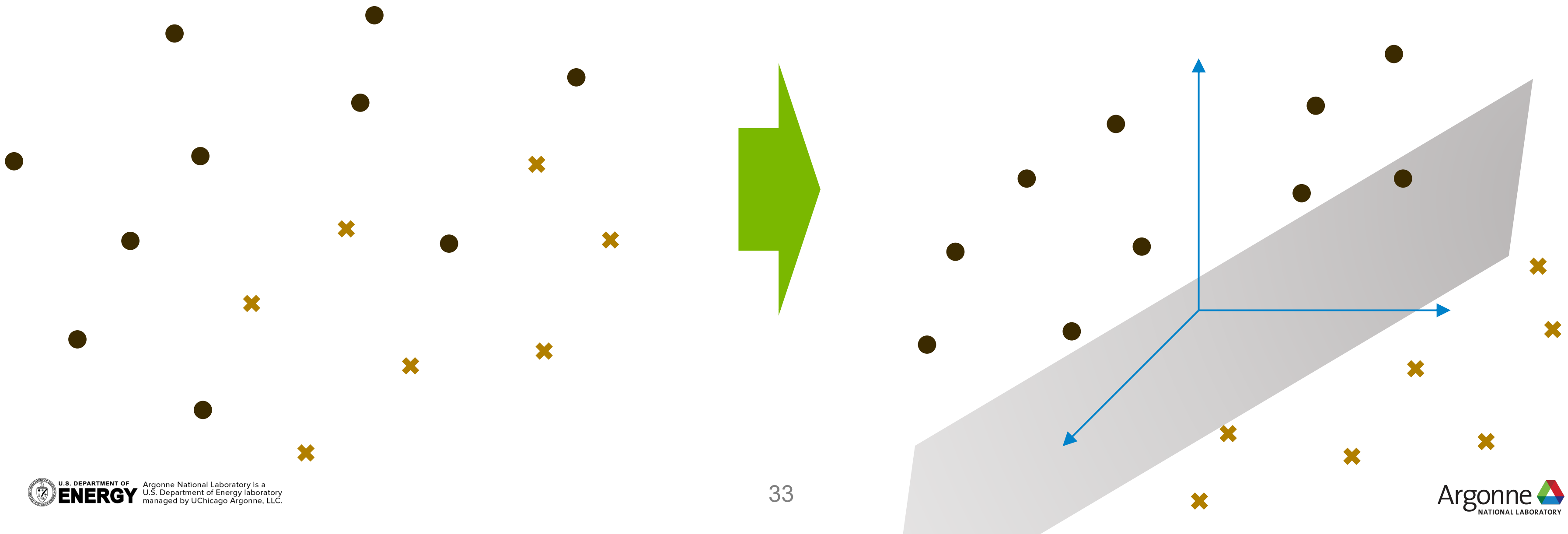
[1] Sergey Bravyi, **Ruslan Shaydulin**, Shaohan Hu, Dmitri Maslov. Clifford Circuit Optimization with Templates and Symbolic Pauli Gates. arXiv:2105.02291

KERNEL METHODS

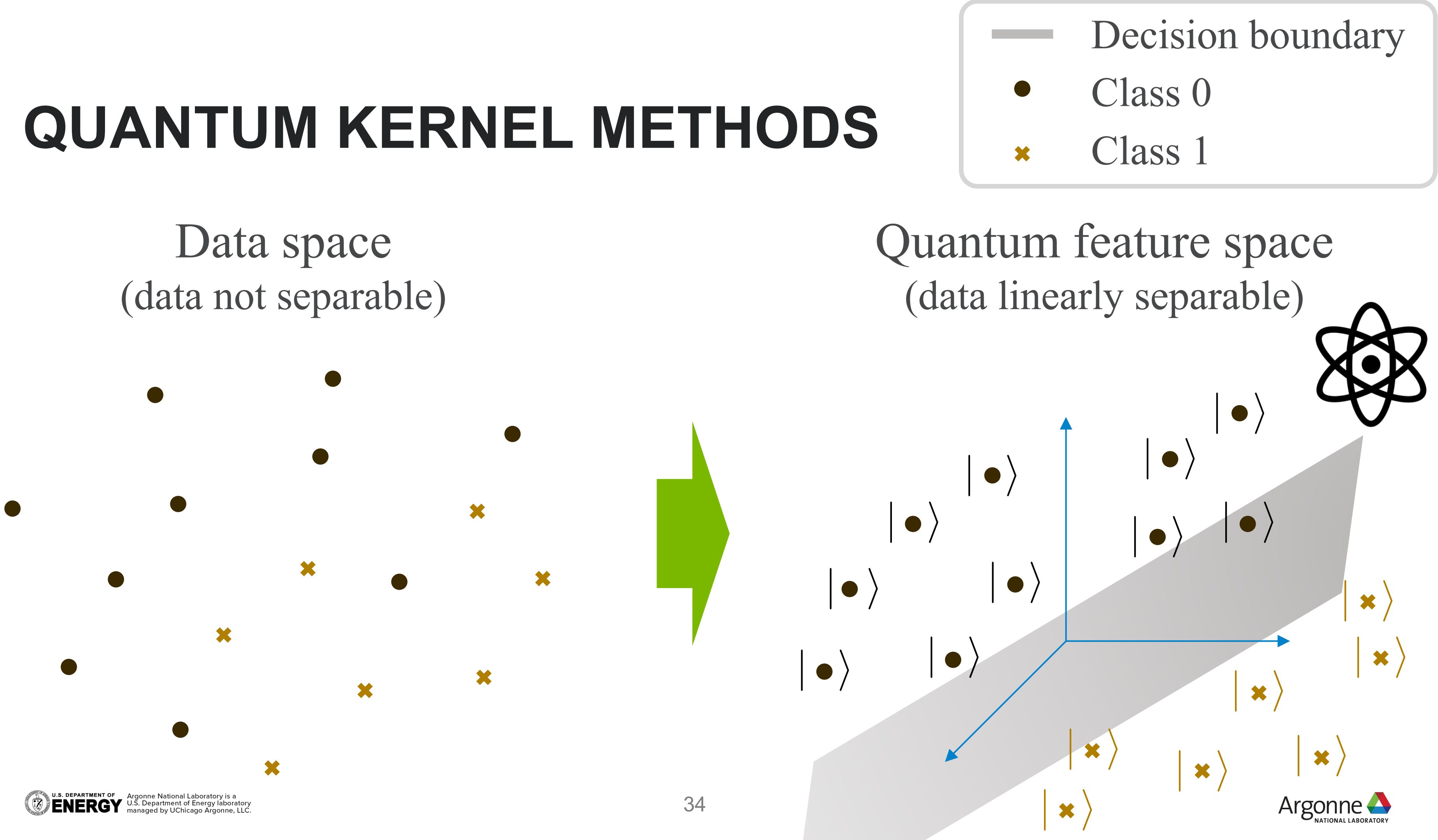


Data space
(data not separable)

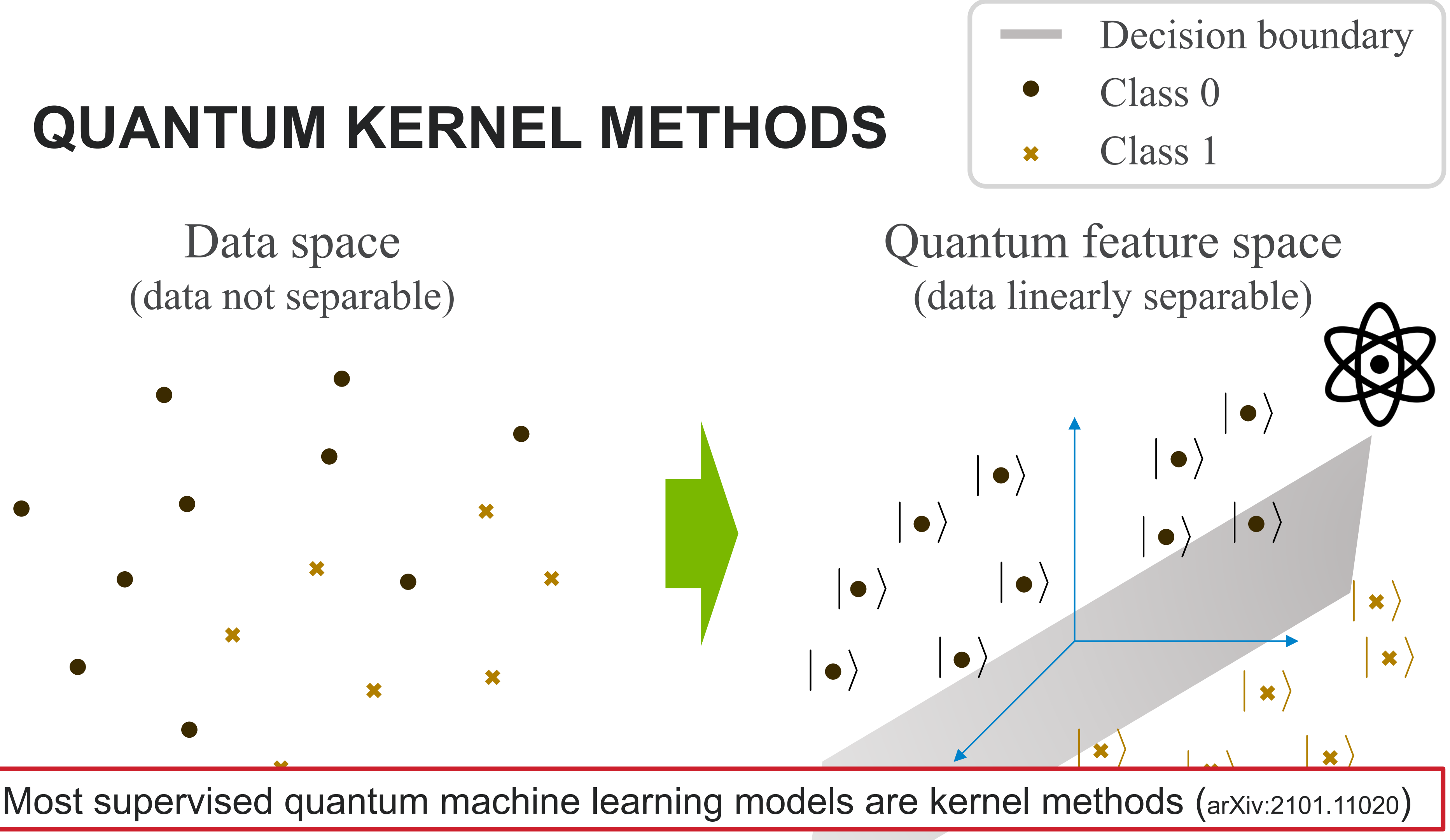
Feature space
(data linearly separable)



QUANTUM KERNEL METHODS

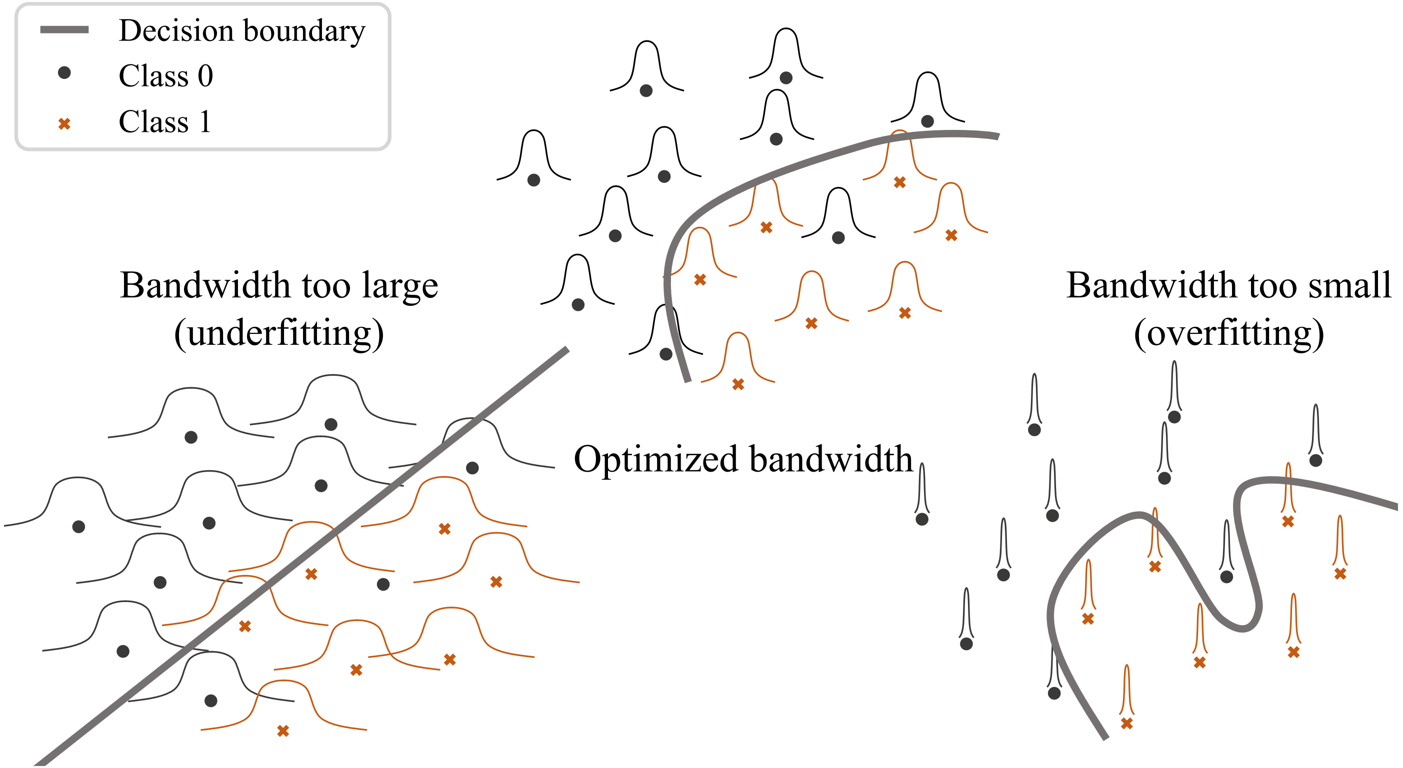


QUANTUM KERNEL METHODS



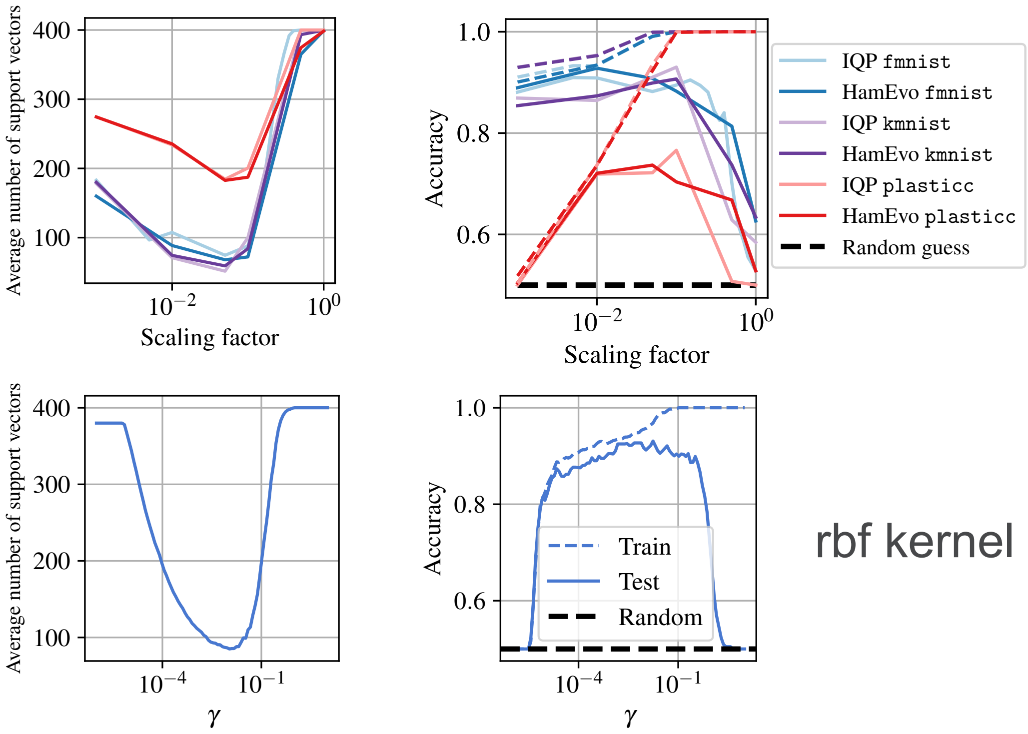
Most supervised quantum machine learning models are kernel methods (arXiv:2101.11020)

IMPORTANCE OF BANDWIDTH IN QUANTUM MACHINE LEARNING



UNDER- AND OVERFITTING IN QML

- Varying quantum kernel bandwidth controls the expressivity of the model
- Consistent behavior across multiple kernels and datasets
- Analogous to classical rbf kernel

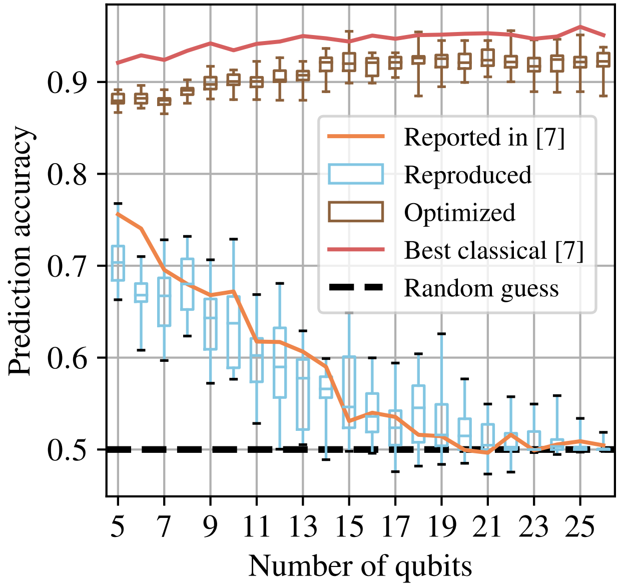


rbf kernel

OPTIMIZING BANDWIDTH IMPROVES PERFORMANCE

From random guess to state-of-the-art

- We reproduce results from recent Google paper [7] that considers the feature map fixed
- Optimizing bandwidth leads to performance comparable to best classical methods!

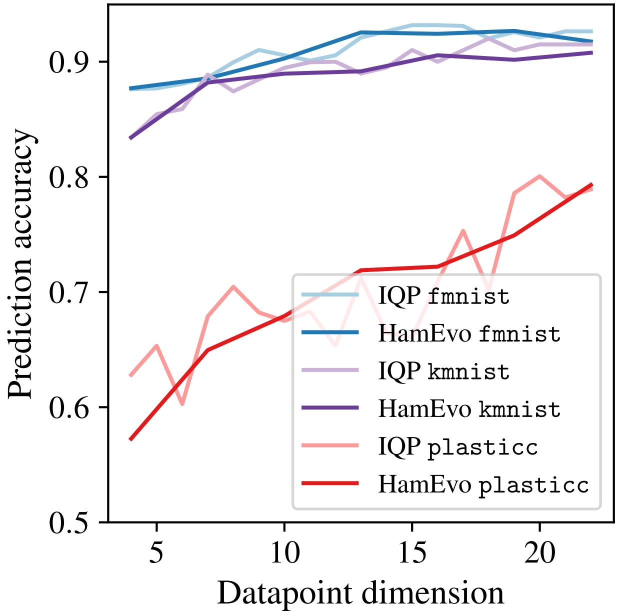


[7] doi: 10.1038/s41467-021-22539-9

arXiv:2111.05451

PERFORMANCE IMPROVES WITH QUBIT COUNT

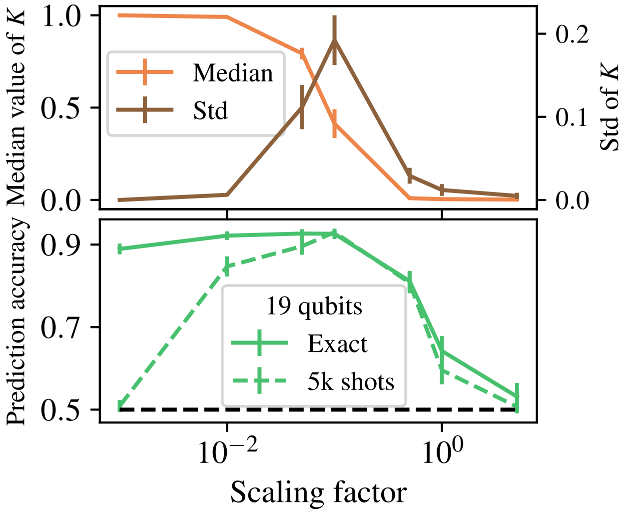
- Previous results show QML performance decrease with qubit count [7]
- With optimized bandwidth, performance improves with qubit count
- No apparent obstacles to quantum advantage from exponential dimensionality of Hilbert space

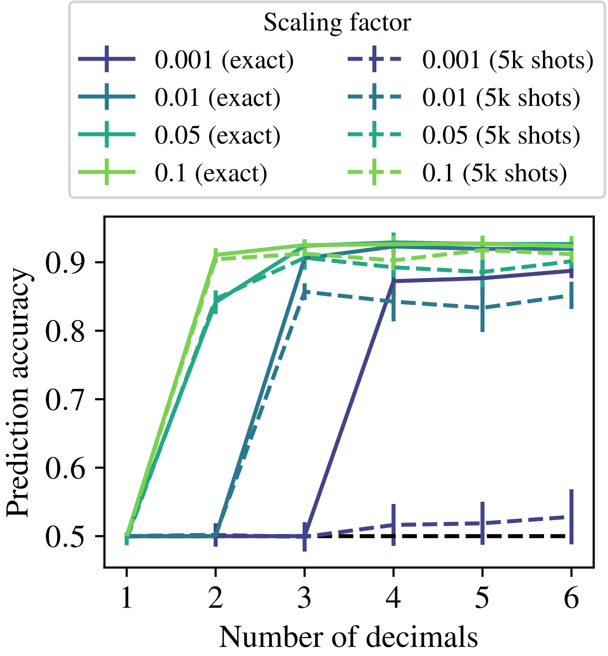


[7] doi: 10.1038/s41467-021-22539-9

arXiv:2111.05451

NO OBSTACLES FROM LIMITED PRECISION AND FINITE SAMPLING





- Observed high performance can be achieved even with limited control precision and sampling noise

REFERENCES

- Error mitigation for QAOA:
  - **Ruslan Shaydulin**, Alexey Galda. Error Mitigation for Deep Quantum Optimization Circuits by Leveraging Problem Symmetries. *2021 IEEE Intl. Conf. on Quantum Computing and Engineering (to appear)* arXiv:2106.04410
- More details on the role of symmetry in QAOA:
  - **Ruslan Shaydulin**, Stefan M. Wild. Exploiting Symmetry Reduces the Cost of Training QAOA. *IEEE Transactions on Quantum Engineering (DOI: 10.1109/TQE.2021.3066275)* arXiv:2101.10296
  - **Ruslan Shaydulin**, Stuart Hadfield, Tad Hogg, Ilya Safro. Classical symmetries and QAOA. *Quantum Information Processing (DOI: 10.1007/s11128-021-03298-4)*. arXiv:2012.04713
- Quantum kernel bandwidth:
  - **Ruslan Shaydulin**, Stefan M. Wild. Importance of Kernel Bandwidth in Quantum Machine Learning. *(in submission)* arXiv:2111.05451